

Spatially resolved THz response as a characterization concept for nanowire FETs

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Abstract—In this paper, we propose a THz probe technique to obtain spatially resolved information about the electronic spectra inside nanowire-based FETs. This spectroscopic approach employs a segmented multi-gate design for the local detection of quantum transitions between few-electron states within the FET channel. We simulate the intra-band THz response of such devices by means of a many-body quantum approach, taking quantization and Coulomb interaction effects into account. The obtained simulation results demonstrate the capabilities of the proposed technique which go beyond the limitations of standard characterization methods.

I. INTRODUCTION

The electronic properties of ultimately scaled nanotransistors are dominated by only a handful of electrons or holes. In such nanodevices, one has to face two non-classical physical mechanisms. Firstly, due to the spatial confinement of charge carriers on a nanoscale, quantization energies of electronic states become relevant, leading to a non-classical transport behavior. Secondly, the details of the Coulomb interaction between the individual carriers become important and can no longer be described in terms of a classical mean-field picture. The consequences can be clearly observed experimentally for example in Coulomb blockade phenomena.

One-dimensional nanowire-based field effect transistors (FET) have recently attracted great interest due to their advantageous electrostatics and transport properties [1], [2], [3]. From a different perspective, they also represent prototypes for the study of technological as well as physical challenges in future transistor designs. Instead of considering quantization and Coulomb phenomena as unwanted deviations from the classical device behavior, here one actually utilizes such non-classical effects for the improvement of FET devices or for new functionalities in a future quantum information technology.

In order to understand and finally utilize the physics of quantization and Coulomb effects within such nanowire FETs, one needs a characterization technique that is able to probe quantum states. Typical quantum energy scales of few-electron states in realistic nanowire FETs are on the order of a few meV corresponding to the 100GHz-1THz frequency range. We therefore propose the concept of a spatially resolved THz probe to directly measure quantum transitions between few-electron (or -hole) states within a nanowire FET. This

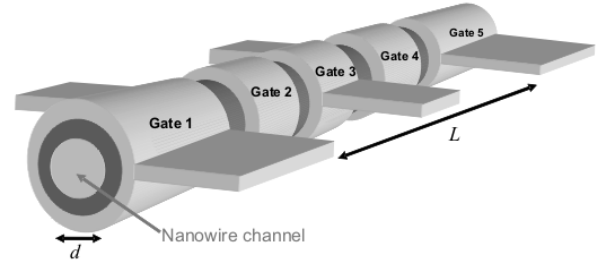


Fig. 1. Schematic view of an idealized nanowire MOSFET in multi-gate configuration ("caterpillar FET"). This example shows a system with 5 gates. Here, gates 1 and 5 are negatively biased and thus provide barriers. Gates 2,3,4 cover a channel region of length L and act as probes. In the simulations, the inter-gate gaps are assumed to be negligible. The outer source and drain contacts are not shown here.

spectroscopic approach employs a multi-gate FET layout, thus being able to provide spatially resolved information about the electronic spectra and electronic charge distributions inside the FET channel. Such a concept goes beyond the capabilities of standard linear and nonlinear characterization methods [4]. In this paper, we discuss the theoretical aspects of the proposed multi-gate THz probe. We simulate the intra-band THz response of nanowire FET devices by means of a many-body quantum approach, taking quantization and Coulomb interaction effects beyond mean-field into account.

In the following sections, we first describe the main physical ideas behind our many-body THz simulation approach, and secondly, we demonstrate the strengths of the concept of a THz probe by discussing a realistic example of a multi-gate nanowire FET. As a main effect, we obtain the formation of a Wigner molecule in the long channel limit.

II. THEORETICAL APPROACH

Fig. 1 shows a schematic sketch of the considered nanowire FET with multiple gate segments. We assume that only one lateral subband needs to be taken into account, corresponding to channel diameters in the sub-30 nm range for GaAs. In order to capture the numerous details of a real device structure, such as the actual geometrical configuration of the gate electrodes, a realistic quantum simulation of such a nanodevice requires the consideration of a sufficiently large number $Z \approx 50 - 500$

of single-particle states [5], [6]. In contrast to the commonly employed Anderson- or Hubbard-like many-body models [7], [8], in general we have to account for an inhomogeneous, anisotropic, and screened Coulomb interaction. Since the resulting many-body problem scales exponentially in Z , such a realistic simulation thus grows beyond any computational limit. In this context, we have recently introduced a multi-configurational approach (MCSCG, [3], [9], [10]) which employs a reduced adaptive basis for the simulation of Coulomb blockade phenomena in nanowire FETs. For the simulation of THz response, however, the number of considered basis states has yet to be increased. As a solution, we have therefore extended the MCSCG by a “bucket-brigade” algorithm (BBCI) [11], [12] which allows us to select a few thousand relevant many-body configurations from the exponentially growing basis set. A general few-electron state in turn can be written as a linear combination of such relevant configurations. This approach enables us to describe correlated many-body states beyond mean-field theory (e.g. Hartree-Fock or LDA-DFT [13]) which become essential within the field of quantum information technology. The following simulation results are based on the BBCI algorithm in combination with first-order Kubo theory [14] for the description of the THz response spectra within the chosen relevant many-body basis.

III. SIMULATION RESULTS

For the following idealized example, the outer ends of the channel are covered by gate electrodes (for example gates 1 and 5 in Fig. 1). Applying a sufficiently large negative voltage to the outermost gates, barriers arise and we thus can assume an almost isolated channel system. The input THz excitation is applied to gate 1 (see Fig. 1), whereas the intermediate gate fingers (gates 2,3,4 in Fig. 1) serve as spatially resolved probes with zero DC bias. In our example, we consider two different GaAs-based nanowire MOSFETs with SiO_2 shell and $40 + 2$ gate segments. In both cases we keep the channel diameter $d = 20\text{nm}$ and the oxide thickness $d_{ox} = 10\text{nm}$ constant, whereas the channel lengths are chosen as $L = 150\text{nm}$ and $L = 600\text{nm}$ with corresponding total oxide capacitances of $C_{ox} = 47\text{aF}$ and $C_{ox} = 188\text{aF}$, respectively. Due to the coaxial gate electrodes, the Coulomb interaction within the channel region is strongly screened. In the considered example, we obtain a screening length [15], [3] of $\lambda = 10.5\text{nm}$ for $\epsilon_{ox} = 3.9$ and $\epsilon_{ch} = 12.4$. In the following discussion, we assume a thermodynamical equilibrium state in the low temperature limit in order to obtain a well-resolved occupation of quantum states. The total electron number is kept fixed at $N = 4$, trapped within the inner channel region L . As for a possible experimental preparation of such an electronic state, one could employ the outer source and drain contacts in combination with suitable barrier-gate voltages to make use of single-electron tunneling for electron counting [16].

Fig. 2 shows the simulated charge density along the channel axis for the nanowire FET with $L = 150\text{nm}$. For comparison, the non-interacting case is shown in Fig. 2(a), whereas the realistic case which includes the Coulomb repulsion is plotted

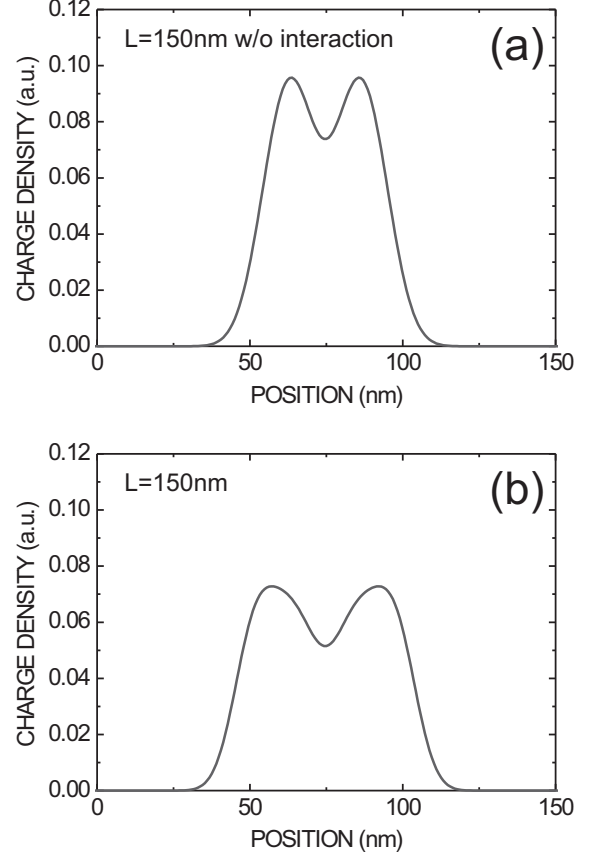


Fig. 2. Simulated electron charge density for a GaAs nanowire FET with $L = 150\text{nm}$ and $d = 20\text{nm}$. The number of electrons is $N = 4$. (a) shows the non-interacting case, whereas (b) includes the electron-electron interaction. Comparing the two cases, no significant qualitative change can be observed.

in Fig. 2(b). For this case, the single-particle quantization energy dominates as compared to the Coulomb repulsion, resulting in a charge distribution which resembles the shape of a non-interacting system. Here, the Coulomb repulsion solely broadens the spatial electron distribution. In contrast, for the $L = 600\text{nm}$ case (Fig. 3(a) and (b)) one can clearly identify the formation of a charge density wave, indicating the onset of the Wigner molecule regime [17] with separated electrons owing to the dominating Coulomb repulsion. The actual transition to the Wigner regime for a nanowire FET in general results from a competition between kinetic energy and Coulomb energy, which of course depends on the chosen materials and geometries. In the long-channel case ($L = 600\text{nm}$), the mean spatial separation of the electrons $\Delta x \simeq L/N$ becomes much larger than the screening length λ of the Coulomb interaction within the channel. For the discussed example, in turn, it is energetically favorable for the electrons to form a charge density wave in order to reduce the Coulomb energy, outweighing the increased kinetic energy due to the spatial confinement Δx . Comparing the non-interacting case Fig. 3(a)

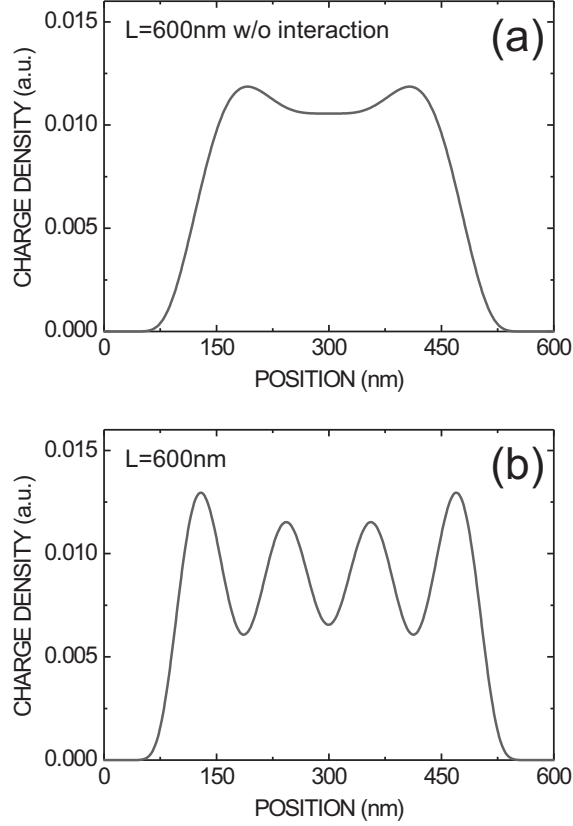


Fig. 3. Simulated electron charge density for a GaAs nanowire FET with $L = 600\text{nm}$ and $d = 20\text{nm}$. The number of electrons is $N = 4$. (a) shows the non-interacting case, whereas (b) includes the electron-electron interaction. The charge-density wave in (b) indicates the formation of a Wigner-molecule within the long-channel device. Here, the electron density differs qualitatively from the non-interacting case (a).

with Fig. 3(b), one can clearly observe a qualitative change in the electron density profile.

In order to probe such a peculiar electronic configuration within a nanowire FET channel, we now consider the spatially resolved THz response spectrum of such a device. In the following simulation results, we have employed a resolution of 40 intermediate probe gates. One has to note that each individual gate finger detects a spatially averaged signal within an effective interval $l_G^{eff} \simeq l_G + 2\lambda$, where l_G denotes the geometrical length of the gate segment and λ the gate screening length. Parasitic stray-capacitances which will likely occur in an experimental realization of such a device are not considered in this paper. For the experimental case it might be advantageous to employ alternating screening and signal gates, combined with an optimized THz layout.

Fig. 4 and Fig. 5 show the simulated THz spectra for the two cases $L = 150\text{nm}$ and $L = 600\text{nm}$, respectively, which exhibit fundamental resonances at 1.69THz and 70GHz. The higher value for the 150nm case stems from a narrower electron distribution (see Fig. 2(b)). Most noticeably, comparing the

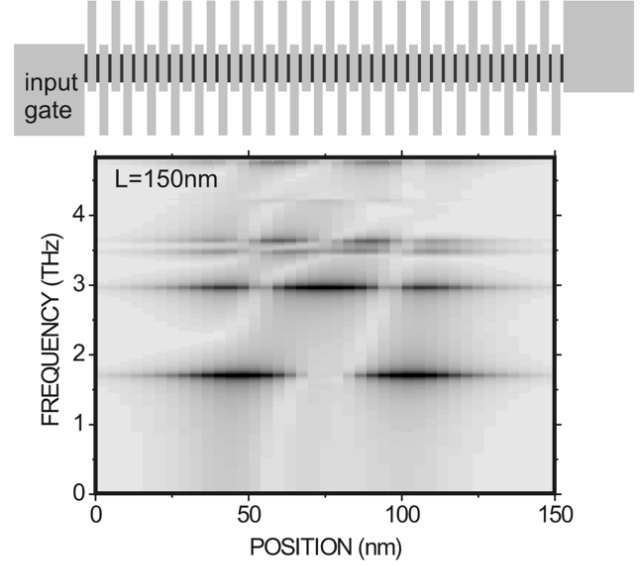


Fig. 4. Top-view of the nanowire FET (40+2 gates) and the simulated THz transition spectrum for a GaAs nanowire with $L = 150\text{nm}$ and $d = 20\text{nm}$. The number of electrons is $N = 4$. Within the grayscale plot, black corresponds to a strong response signal. For this device, the main effect of the electron-electron interaction consists mainly in a renormalization of the energy spectrum.

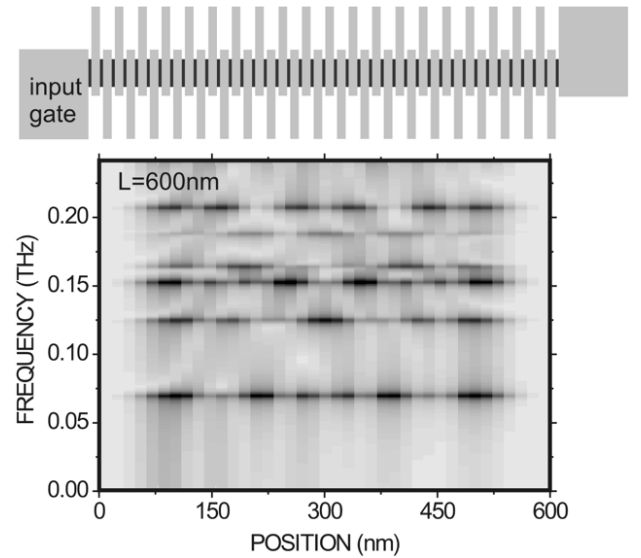


Fig. 5. Top-view of the nanowire FET (40+2 gates) and the simulated THz transition spectrum for a GaAs nanowire with $L = 600\text{nm}$ and $d = 20\text{nm}$. The number of electrons is $N = 4$. Within the grayscale plot, black corresponds to a strong response signal. As compared to the short-channel case in Fig. 4, the formation of a Wigner-molecule leads to additional spatial peaks.

qualitative form of the two spectra, signatures of the Wigner-like regime for the 600nm case (Fig. 5) can be identified via the appearance of additional spatial peaks which are related to the oscillatory nature of the charge density wave. One has to note that the maxima in these transition spectra are located at those gate positions where the charge *oscillates* the most, and thus need not coincide with the charge density maxima. In fact, for a non-interacting case, the spatial THz pattern is related to the gate-averaged *product* of the two wavefunctions of the involved final and destination states [12]. Even with the inclusion of the electron-electron interaction, the considered $L = 150\text{nm}$ device comes close to such a situation. In the case of a correlated many-body state, however, such an interpretation is not applicable in general and a many-body approach such as the BBCI becomes mandatory. In any case, the obtained THz spectra can be considered as “fingerprints” of the concrete electronic configuration of the channel, providing not only information about electronic transition energies but also about the spatial configuration of the underlying few-electron states.

IV. CONCLUSION

In summary, we have considered a THz probe for a spatially resolved analysis of electronic spectra in nanowire-based transistors employing a multi-segment gate design. We have simulated the THz response of few-electron quantum states in nanowire FETs by use of a recently developed numerical many-body technique. The discussed example of a GaAs-based device demonstrates that signatures of Wigner-like charge density waves can be identified by use of this method, which lies beyond the scope of standard FET characterization methods. As such, the proposed multi-gate THz probe technique might prove useful in a future experimental realization as a means to characterize nanoscale devices which are dominated by quantization and Coulomb effects.

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